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Localization aspect of electron phonon-coulomb system.

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Localization aspect of electron-phonon-coulomb (EPC) system has been discussed on the basis of continuum approximation. The condition for localized state for such system has been derived and it is found that for a stable localized state $W_0^r \geqslant 0{\cdot}008\ \hbar\omega_q$, where W_0^r is the electronic ground state energy in the localized state and ω_q is the re-normalized phonon frequency and that there exists a meta-stable zone prescribed by $-1{\cdot}2\ \hbar\omega_q < W_0^r < 0{\cdot}008\ \hbar\omega_q$ Expressions for electronic mobility have been deduced and the results obtained shows that the overall effect of the coulomb interaction is to increase the electronic mobility.

1 Introduction

The electron localization aspect related to the electron-phonon (EP) system has been extensively studied both theoretically and experimentally during the past two decades (Yamashita & Kurosawa 1958, Bogomolov & Kudinov 1968, Austin & Mott 1969, Austin 1972, Sumi 1972), and the many important results obtained enhanced our knowledge about the form of interaction existing in solids. The effect of coulomb interaction on the localization aspect was not examined chiefly because the localized states of electron in an EPC system are largely modified and one finds a lot of difficulty in obtaining an accurate quantitative estimate of this modification. The principal objective of the present paper is to construct a theoretical framework regarding the electron localization aspect of an EPC system. In constructing such a formulation, we are primarily interested in finding out an appropriate approximation for the energy spectrum of the system. The continuum approximation has been shown by simple reasonings to be a suitable method for studying the present problem. This technique is, however, more applicable to an EPC system than to an EP system. The advantage of continuum approximation is that several important aspects including the localization problem for an EPC system can be treated very satisfactorily. The quasi-particle spectra of an EPC system has been briefly described here on the basis of this approximation The condition for a delocalized or bloch state of an electron has been derived and examined critically to observe the effect of coulomb interaction on EPC system. This condition has been found to be of the form, $W_0^r \geqslant 0{\cdot}008\ \hbar\omega_q$, where ω_q is the renormalized phonon energy and

W_0^r is the electronic ground state energy. Localization has been found to depend appreciably upon temperature (when the system is at ordinary temperature), but at low temperatures, localization is essentially temperature dependent. There exists also a meta-stable range, as in an EP system, and this range has been approximately traced out. The effect of coulomb interaction on the electronic mobility in the localized state has also been briefly discussed.

2. Continuum Approximation and Electron Self-Energy

For an EP system, electron trapping by lattice vibration is conceived as follows : the fluctuating potential due to lattice vibrations is regarded as a static short-range potential with the strength distributed at each lattice site in the crystal. An excess electron in the conduction band is trapped within this potential well situated at each lattice site such that the potential energy is lowered. It is, therefore, evident that the magnitude of the electron-phonon coupling determines the depth of the potential well. For a well-localized state, the potential well should be sufficiently deep so that the potential minima at the lattice sites may be assumed to be separated from each other. In other words, the correlated scattering due to several lattice sites can be ignored This basic physical reasoning is adopted in an adiabatic approximation to interpret several important features of electron localization in an EP system.

When we consider the effect of coulomb interaction between two electrons, the most important effect of this interaction is to diminish the electron-phonon coupling. As a result of this the depth of the potential well situated at each lattice site decreases. The electrons well localized within the potential wells in absence of coulomb-interaction, tend to fly off from the respective potential well in presence of this interaction Such an intrinsic delocalization aspect of an EPC system indicates that the continuum approximation is more appropriate for the EPC system than for the EP system; the adiabatic approximation which has been stated as a reasonable approximation for an EP system is not an adequate approximation for an EPC system.

Let us consider the Hamiltonian for an EPC system in the following well-known form

$$H = H_{ph} + H_M \qquad \ldots (1)$$

where H_{ph} is the bare phonon part given by

$$H_{ph} = \sum_{q<q_m} \omega_q^0 a_q^+ a_q \qquad \ldots (2)$$

and H consists of three parts,

$$H_M = H_{el} + H_{coul} + H_{el-ph} \qquad \ldots (3)$$

where H_{el}, H_{coul}, and H_{e-ph} are respectively the bare electron part, coulomb part and electron-phonon part given by

$$H_{el} = \sum_{k} \epsilon_k{}^0 C_k{}^{\dagger} C_k \qquad \ldots (4)$$

$$H_{coul} = \sum_{k_1 k_2 k_3 k_4} V(K_1 K_2 K_3 K_4) C_{k_1}{}^{\dagger} C_{k_2}{}^{+} C_{k_3} C_{k_4} \qquad \ldots (5)$$

$$H_{el-ph} = \sum_{q, k_1, k_2} \alpha^0(q)[a_q(K_1 K_2) + a_q(K_1 K_2)^{+}] C_{k_1}{}^{+} C_{k_2}. \qquad \ldots (6)$$

In the above expressions a_q's and C_k's are phonon and electron creation and annihilation operators, $\omega_q{}^0$ is the bare phonon energy and $\epsilon_k{}^0$ is the bare electron energy, $\alpha^0(q)$ being the unrenormalized electron-phonon coupling constant given by

$$|\alpha^0(q)|^2 = \frac{4\pi e^2}{\Omega q^2} \cdot \omega_q{}^0/2. \qquad \ldots (7)$$

The expression for polarization propagator is

$$D^{-1}(q, \omega) = \{V(q) + I^0(q, \omega)\}^{-1} - \pi \qquad \ldots (8)$$

where π is the irreducible polarization part and $D^0(q, \omega)$ is the bare phonon propagator given by,

$$I^0(q, \omega) = \frac{2\omega_q{}^0 |\alpha^0(q)|^2}{\omega^2 - \omega_q{}^{02} + i\eta}. \qquad \ldots (9)$$

Within the validity of Migdal's theorem, we can easily extract the real and imaginary parts of electron self-energy by using the continuum approximation. Real and imaginary parts are obtained in the form (Chakraborty 1973)

$$\Sigma_0(K, \omega) = -\frac{\alpha_r{}^2 \omega^c}{\Omega} \ln \frac{\omega_q + \omega}{} + O(\omega_q{}^{-2}) \qquad \ldots (10)$$

$$\Sigma_I(K, \omega) \neq -\frac{\alpha_r{}^2 \omega \pi}{2} \operatorname{sgn} w_q + O(\omega_q{}^{-2}), \text{ for } \omega < |\omega_q| \qquad \ldots (11)$$

$$= -\frac{\alpha_r{}^2 \omega^2}{\omega_q{}^2}, \quad \text{for } \omega < |\omega_q| \qquad \ldots (12)$$

where $\alpha_r{}^2$ is the renormalized coupling parameter given by

$$\alpha_r{}^2 = \frac{2\omega_q |\alpha(q)|^2 N(O)}{\Omega}. \qquad \ldots (13)$$

Graphical analysis of the spectral weight function shows up several important features (Chakraborty 1973) One important feature observed is that the quasi-particle peak at $\epsilon_k/(1+\alpha_r^2)$ may be regarded as that corresponding to an electron immersed in an environment of virtual phonon cloud, that is, to an electron trapped by lattice vibration. α_r^2 is greater for an EP system than for an EPC system. This suggests that the quasi-particle peak occurs for much greater energy in the case of an EPC system. This shifting of the quasi-particle peak offers a convincing evidence for introducing the concept of delocalization tendency of an EPC system and lends further support in adopting the continuum approximation.

3 Stable Localized States and Meta-Stable Zone

Let us consider an excess electron in the conduction band coupled to other electrons by coulomb interaction and interacting with the fluctuating lattice polarization field. Such a system is described by the Hamiltonian, $H = H_{ph}+H_M$. In the absence of coulomb interaction H_M consists of two parts : a bare electron part and the other part representing the electron-phonon interaction In adiabatic approximation, the electron-phonon interaction is regarded diagonal with respect to site indices. Such diagonal representation stems from the assumption that the effect of phonons on electrons can be described by a short-range potential fluctuating at each lattice sites. Such a description however, becomes meaningless when the coulomb interaction is taken into consideration because scattering due to several lattice sites cannot be ignored. Such correlated scattering is implicitly included in the continuum approximation as stated earlier Utilising the electron self-energy expressions obtained on the basis of the continuum approximation one can very easily discuss the localization aspect of an EPC system by statistical-mechanical approach in which one introduces the grand canonical partition function and divides into two zones : localized and continuum zones. The usual procedure is to write down the grand canonical partition function in the form,

$$Z = Z_{ph} Z_M \qquad \ldots \quad (14)$$

where Z_{ph} corresponds to the bare phonon part and Z_M to the complicated coupled part wherein the bare electron part, coulomb interaction part and the electron-phonon interaction part are mixed up The coupled part of the partition function can be written as,

$$Z_M = < Tr_{el}\, e^{-\beta H_M} > \qquad \ldots \quad (15)$$

and

$$Z_{ph} = Tr_{ph}\, e^{-\beta H_{ph}}. \qquad \ldots \quad (16)$$

The symolb $< >$ denotes the statistical average over different phonon states. Imaginary part of the electronic Green's function may be written as

$$\text{Im } G(\omega) = -\pi < Tr_{el}\delta(\omega - H_M) >. \quad \ldots \quad (17)$$

Hence the partition function, Z_M, can be expressed in the form

$$Z_M = -\frac{1}{\pi}\int_{-\infty}^{\infty} e^{-\beta\omega}\ \text{Im } G(\omega)d\omega \quad \ldots \quad (18)$$

Expanding $G(\omega)$ in the form,

$$G(\omega) = G_0(\omega) - G_0'(\omega)\,\Sigma(\omega) + \ldots \quad \ldots \quad (19)$$

where $G_0(\omega)$ is the Green's function corresponding to the unperturbed lattice and $G_0'(\omega)$ is its first order derivative. We assume

$$\text{Im } G_0(\omega) \neq 0, \text{ for } |\omega| < \omega_q$$

$$= 0, \text{ elsewhere.} \quad \ldots \quad (20)$$

Then the partition function can be written as,

$$Z_M = Z_M{}^{<} = Z_M{}^{>} \quad \ldots \quad (21)$$

where the two parts are given by

$$Z_M{}^{<} = -\frac{1}{\pi}\int_{|\omega|<\omega_q} d\omega\, e^{-\beta\omega}\ \text{Im } G_0(\omega) \quad \ldots \quad (22)$$

$$Z_M{}^{>} = \frac{1}{\pi}\int_{|\omega|>\omega_q} d\omega\, e^{-\beta\omega} G_0'(\omega) I_m\Sigma(\omega). \quad \ldots \quad (23)$$

Eq. (22) corresponds to the continuum zone and gives rise to broad band spectrum, and eq. (23) gives rise to localized zone. For localization problem, the discussion of eq. (23) is only useful. We consider the Green's function corresponding to the unperturbed lattice,

$$G_0(\omega) = (\omega - \varepsilon_k{}^0)^{-1}. \quad \ldots \quad (24)$$

Replacing the sum by an intregal we get,

$$G_0'(\omega) \simeq \frac{\partial}{\partial\omega}\left[\frac{2^{\frac{1}{2}}.m^{3/2}.\omega^{\frac{1}{2}}}{\pi^2}\right]\int_0^{\omega_q/\omega}\frac{x^2dx}{\sqrt{1-x}}. \quad \ldots \quad (25)$$

where $x = \epsilon_k^0/\omega$. Since $x < 1$, the above expression becomes

$$G_0'(\omega) \simeq -\frac{2^{3/2}.m^{3/2}.\omega_q^{3/2}}{\pi^2\omega^2}\left[\frac{2\omega_q}{5\omega} + \frac{1}{3}\right] \quad \ldots (26)$$

Therefore, the partition function corresponding to the localized zone reduces to,

$$Z_M^> = (2m^3\omega_q)^{\frac{1}{2}}\frac{\alpha_r^2}{3\beta\pi^3}\left[e^{-\beta W_0^r} + \frac{6\pi^{\frac{1}{2}}\beta\omega_q}{5}\mathrm{erfc}(\beta W_0^r)^{\frac{1}{2}}\right] \quad \ldots (27)$$

where W_0^r refers to the minimum energy of the quasi-electron required for its localization, and erfc(x) is an error function given by,

$$\mathrm{erfc}(x) = \frac{2}{\pi^{\frac{1}{2}}}\int_x^\infty \exp(-u^2)du. \quad \ldots (28)$$

For large positive value of βW_0^r we can write,

$$Z_M^> = N_s\, e^{-\beta W_0^r} \quad \ldots (29)$$

where N_s may be termined as the localization factor given by the following expressions,

$$N_s = \frac{(2m^3\omega_q)^{\frac{1}{2}}\alpha_r^2}{3N\beta\pi^3}\left(1+\frac{6\omega_q}{5W_0^r}\right) \quad \ldots (30)$$

N being the number of electrons per unit volume. For N to become large zero, we should have

$$W_0^r = -1{\cdot}2\hbar\omega_q \quad \ldots (31)$$

which may be regarded as the condition for delocalization

For EPC system, the renormalized phonon frequency can be represented in the form,

$$\omega_q \cong \omega_q^0(1+F/4) \quad \ldots (32)$$

F being the Fröhlich's coupling parameter. Replacing ω by its unrenormalized value (EP system),

$$\omega'_q \cong \omega_q^0(1-F/4) \quad \ldots (33)$$

we obtain the condition for localized state for EP system,

$$W_0 = -1{\cdot}2\hbar\omega_q^0(1-F/2). \quad \ldots (34)$$

Comparing eqs. (31) and (34), we get,

$$W_0^r < W_0,$$

which brings forth the most significant result that the effect of coulomb interaction is to prevent the electron from being localized at a lattice site.

Several other peculiar features are to be observed from the expression for N In the first place, contrary to the usual belief, N depends on temperature both for the EP and the EPC systems Dependence on temperature, although a new feature, has, however, some physical meaning Since N is practically regarded to have its contribution from the vibrational states associated with the localized quasi-electrons, and since the vibrational states can implicit temperature dependence, the fact that the localization factor depends on temperature cannot be considered to be physically inconsistent. Another unconventional feature is that, even at ordinary temperature, N is less than unity, which implies that for well-localized state W_0^r must be very small. At about 300°K, we have $W_0^r \simeq 0{\cdot}008\ \hbar\omega$, for N_s to become unity The physical meaning of this result is as follows. For $W^r{}_0 < 0\ 008\ \hbar\omega$, the localization factor becomes greater than unity Now, decrease of $W^r{}_0$ corresponds to the increase of electron-phonon coupling, and as the latter increases, localization becomes more favourable and thus the result that N_s becomes greater than unity as W_0^r becomes smaller, does not go against the physical reasoning It is to be noted further that when W_0^r is comparable with the phonon energy, localization occurs at abnormally high temperatures, of the order of 10^7 °K but at this high temperature, lattice structure breaks down and the solid transforms to the gaseous state. Consequently, the electron localization by lattice polarization field at this stage is physically inconcievable On the other hand, at sufficiently low temperatures, say, below liquid helium range, the localization factor does not vary appreciably with temperature, but since at these temperatures, electron-phonon coupling is very weak, the temperature dependence as far as the localization is concerned is not important.

It would be interesting to point out that the two conditions which we have derived,

1) $W^r{}_0 = -1{\cdot}2\ \hbar\omega_q$, for localization and,

2) $W^r{}_0 \doteq 0{\cdot}008\ \hbar\omega_q$, below which localization factor > 1 denonstrates the fact that there exists a meta-stable zone prescribed by

$$-1{\cdot}2\ \hbar\omega_q < W^r{}_0 < 0{\cdot}008\ \hbar\omega_q. \qquad \ldots\ (36)$$

Corresponding zone for the EP system can be written as

$$-1{\cdot}2\ \hbar\omega_q(1+F/4) < W^r{}_0 < 0{\cdot}008\ \hbar\omega\ (1+F/4) \qquad \ldots\ (37)$$

4. Effect of Coulomb Interaction on Electronic Mobility

To deduce the expression for electronic mobility related to the EPC system we start from the following expression for the relaxation time, τ, (Sumi 1972),

$$\tau = \tau^{<} + \tau^{>} \qquad \ldots (38)$$

where

$$\tau^{<} = -\frac{\beta}{Z_M^{<} + Z_M^{>}} \int_{|\omega|<\omega_q} d\omega\, e^{-\beta\omega} \frac{K(\omega)}{\mathrm{Im}\,\Sigma(\omega)} \qquad \ldots (39)$$

$$\tau^{>} = \frac{2\beta}{\pi(Z_M^{<} + Z_M^{>})} \int_{|\omega|>\omega_q} d\omega\, e^{-\beta\omega} (\mathrm{Im}\,\Sigma(\omega)^2) \int_{|\omega'|<\omega_q} d\omega' \frac{K(\omega')}{(\omega-\omega')^4} \qquad \ldots (40)$$

The kernel, $K(\omega)$, is given by

$$K(\omega) = \frac{1}{4} \sum_k \left(\frac{\partial\epsilon}{\partial K}\right)^2 \delta(\omega-\epsilon_k) \qquad \ldots (41)$$

Assuming that $K(\omega)$ is extremely small except for $\omega \simeq \epsilon \simeq \omega_q$, we get,

$$K(\omega) \cong (2m^3\omega_q^3)^{\frac{1}{2}}/(5\pi^2). \qquad \ldots (42)$$

Using the expressions,

$$Z_M^{<} = N_c e^{\beta\omega_q}; \quad N_c = (m^k\beta T/2\pi)^{3/2} \qquad \ldots (43)$$

the relaxation time, τ, comes out as

$$\tau = \frac{4\omega_q^{\frac{1}{2}}\beta^{3/2}}{5\pi\alpha_r^2}\left[\frac{\mathrm{erfc}(\beta^{\frac{1}{2}}\omega_q^{\frac{1}{2}}) + (\alpha_r^6/\pi^{\frac{1}{2}})\exp(-\beta W_a)}{\exp(\beta\omega_q) + \frac{4}{3\pi^{3/2}}\left(1+\frac{6\omega_q}{5\overline{W}r_0}\right)\beta^{\frac{1}{2}}\alpha_r^2\omega_q^{\frac{1}{2}}\exp(-\beta W r_0)}\right] \qquad \ldots (44)$$

where W_a represents the activation energy of the hopping of localized electron from one site to another. $\mathrm{erfc}(x)$ is the error function given by,

$$\mathrm{erfc}(x) = \frac{2}{\pi^{\frac{1}{2}}} \exp(-u^2)du. \qquad \ldots (45)$$

Since the mobility is given by $\mu = e\tau/m$, the electronic mobility in the localized state for the EPC system may therefore be written in the form,

$$\mu_{loc} \cong \frac{3e\beta\alpha_r^2}{5m}\left(1+\frac{6\omega_q}{5\overline{W}r_0}\right)^{-1} e^{-\beta(W_a - Wr_0)} \qquad \ldots (46)$$

Replacing ω_q by its unrenormalized value, we observe that for EP system, electronic mobility in the localized state is smaller than μ_{bc} as given above. Thus

the effect of coulomb interaction is to increase the mobility of quasi-electrons in the localized state.

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